Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>

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chain nodes :
11 14 15 16 17 18
                     21 23
ring nodes :
1 2 3 4 5 6 7
ring/chain nodes :
10 12
chain bonds :
2-21 7-10 9-23 10-11 10-12 12-14 15-16 16-17 16-18
ring bonds :
                      4-5 5-9 6-7 7-8
1-2 1-5 2-3
            3-4 4-6
exact/norm bonds :
1-2 1-5 2-3 2-21 3-4 4-6 4-5 5-9 6-7 7-8 8-9 9-23 10-11 10-12 12-14
16-17 16-18
exact bonds :
7-10 15-16
isolated ring systems :
containing 1 :
```

G1:H,[*1]

G2:H,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 21:CLASS 23:CLASS

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1

STR

0

G1 H, [@1]

G2 H,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful

FULL SEARCH INITIATED 06:10:34 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED -

1220 TO ITERATE

100.0% PROCESSED 1220 ITERATIONS

SEARCH TIME: 00.00.01

L2

21 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

21 ANSWERS

166.94 167.15

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 06:10:38 ON 28 APR 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 28 Apr 2006 VOL 144 ISS 18 FILE LAST UPDATED: 26 Apr 2006 (20060426/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> s 12

L3 2 L2

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ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
2005:1171056 CAPLUS
143:440931
Preparation of N-hydroxy pyrrolopyrimidinecarboxamides as inhibitors of HIV integrees.
Dress, Klaus Ruprecht; Hu, Qiyue; Johnson, Ted Milliam; Plewe, Michael Bruno; Tanie, Steven Paul; Wang, Hai; Yang, Anle; Yin, Chunfeng; Zhang, Junhu Pfizer Inc., USA
PCT Int. Appl., 177 pp.
CODEN: PIXXD2
Patent
English
N.CNT 1
PATENT NO. KIND DATE APPLICATION NO. DATE

MO 2005103003 A2 20051103 NO 2005-1B1029 20050414
NO 2005103003 A3 20060316
N; AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CH, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GB, GH, GM, HR, HU, ID, IL, IN, 1S, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, NM, MM, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PT, RO, RU, SC, SD, SE, SG, SK, SL, SK, ST, TJ, TM, TM, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, RM, EM, GH, KE, LS, MN, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZM, AM, AZ, BY, KG, KZ, MD, RU, 10, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, 15, IT, LU, LU, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CT, CM, GA, GN, QG, GM, ML, HR, NE, SN, TD, TG
US 2005-660502P P 20050309
IN
                                                                                                                                                                                                                                                                                                                                                                                                                   US 2004-565705P
US 2005-660502P
US 2005-115003
US 2004-565705P
US 2005-660502P
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            P 20040426
P 20050309
20050425
P 20040426
P 20050309
                                              US 2005277662
                                                                                                                                                                                                                                                                                                    20051215
                                            MARPAT 143:440391
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ı

Title compds. [I; R1 = H, (substituted) alkyl, alkenyl, heteroalkyl; R2, R5 = H; R3 = (CR8R9):NRIORNI, (substituted) heteroalkyl; R4 = H, halo, alkyl, heteroalkyl, (substituted) alkenyl, alkynyl, OR12a, NR12aR12b; R6

H, alkyl, heteroalkyl, (substituted) alkenyl; R8, R9 = H, alkyl; R10R11N

- L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) (substituted) cycloheteroalkyl; R12a, R12b, R12c = H, alkyl; t = 1-3], were prepd. Thus, 1-(2,4-difluorobenzyl)-1H-pyrrolo[2,3-c]pyridine-5-carboxylic acid (prepn. given) was stirred with O-(7-azabenzotrizo21-1-yl)- [1,1,3,3-tetramethyluronium hexafluorophosphate, Et3N, and NH2OH.HCl in
- - for 16 h to give 48% N-hydroxy-1-(2,4-difluorobenzyl)-1H-pyrrolo[2,3-c)pyridine-5-carboxamide. The latter showed an EC50 = 0.00795 μ M in an HIV-1 cell protection assay.

=> d hitstr

ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN 688314-07-0P 868550-24-7P 868550-25-8P 868550-26-7P 868550-27-0P RD: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Usea) (preparation of N-hydroxy pyrrolopyrimidinecarboxamides as inhibitors IV

of HIV

iv integrame)
688314-07-0 CAPLUS
3H-Imidaco(4.5-c)pyridine-6-carboxamide, 3-{(4-fluorophenyl)methyl}-N-methoxy- (9CI) (CA INDEX NAME)

868550-24-7 CAPLUS
3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(4-fluorophenyl)methyl]-N-hydroxy- (9CI) (CA INDEX NAME)

868550-25-8 CAPLUS
3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-{(4-fluorophenyl)methyl]-N-hydroxy-N-methyl- (9CI) (CA INDEX NAME)

RN 868550-26-9 CAPLUS
CN 3H-Imidazo(4,5-c)pyridine-6-carboxamide,
3-[(2,3-difluorophenyl)methyl]-Nhydroxy- (9C1) (CA INDEX NAME)

L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

868550-27-0 CAPLUS
3H-Imidazo(4,5-c)pyridine-6-carboxamide, 3-(2-cyclohexylethyl)-N-hydroxy-(9C1) (CA INDEX NAME)

=> d fbib abs hitstr 2

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN 2004:390246 CAPLUS 140:406796 Preparation of pyrrolo[2,3-c]pyridine hydroxamates as HIV-integrase inhibitors Hu, Qiyue; Kuki, Atsuo; Nowlin, Dawn Marie; Plewe, Michael Bruno; Wang, Hai; Zhang, Junhu Pfizer Inc., USA PCT Int. Appl., 108 pp. CODEN: PIXXD2 Patent L3 AN DN TI IN PA 50 DT Pate... LA English FAN.CNT 1 PATENT NO. DATE DATE 20040513 20040916 APPLICATION NO. KIND A2 20040513 NO 2003-IB4735 20031027
A3 20040916
AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CZ, DE, DK, DW, DZ, EC, EE, ES, FI, GB, GD, GE, GH, LV, MA, MD, MG, MK, MN, MM, MK, MZ, NI, NO, NZ, OM, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TM, TR, TT, US, UZ, VC, VN, YU, ZA, ZH, ZW
RG, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TG, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TC, CG, CI, CH, GA, GN, GO, GM, ML, MR, NE, SN, TD, TG
AA 20040513 CA 2003-2500487 P 20031027
A1 20040525 AU 2003-2500487 P 20031027
A2 20050803 P 2003-751203 W 2001027
A2 20050803 P 2003-751203 W 20031027
A3 20050913 W 2003-184735 W 20031027
A2 2005023 P 2003-751203 W 20031027
A3 200502422513P W 20031027
A3 20050213 W 2002-422513P W 20031027
A4 200508 W 2003-184735 W 20031027
A5 20050233 P 2003-75820 P 20021031
A6 2005-184735 W 20031027
A7 20060233 P 2003-184735 W 20031027
A8 2005-184735 W 20031027
A9 2005-184735 W 20031027 WO 2004039803 WO 2004039803 A2 A3 WO 2003-IB4735 20031027 039803
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CO, CR, CU,
GM, HR, HU,
LS, LT, LU,
PH, PL, PT,
TZ, UA, UG,
GH, GM, KE,
KG, KZ, MD,
FI, FR, GB,
BF, BJ, CF, CA 2500487 AU 2003269421 AT, BE, CH, DE, DK, ES, FR, GB, IE, SI, LT, LV, FI, RO, MK, CY, BR 2003015820 JP 2006506398 US 2004147547 US 2002-422513P P 20021031 MARPAT 140:406796

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) fluorobenzyl)-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-23-0P

fluorobenzyl)-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-23-09

,3-Difluorobenzyl)-N-phenoxy-3H-imidazo[4,5-c]pyridine-6-carboxamide
688314-24-19, 3-(2,3-Difluorobenzyl)-N-methoxy-3H-imidazo[4,5-c]pyridine-6-carboxamide
688314-24-19, 1-(4-Fluorobenzyl)-N-phenoxy-1H-imidazo[4,5-c]pyridine-6-carboxamide
688314-26-39, 1-(4-Fluorobenzyl)-N-phenoxy-1H-imidazo[4,5-c]pyridine-6-carboxamide
688314-25-59, N-Methoxy-3-(2,3-difluorobenzyl)-3H-imidazo[4,5-c]pyridine-6-carboxamide
688314-29-59, N-Methoxy-3-(3-methylbutyl)-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-29-69, 3-(2-dyclohexylethyl)-N-phenoxy-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-39-69, 3-(3-methylbutyl)-N-phenoxy-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-39-19, N-Allyloxy-3-(2-cyclohexylethyl)-N-phenoxy-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-31-3P, N-Allyloxy-3-(2-cyclohexylethyl)-N-Phenoxy-3H-imidazo[4,5-c]pyridine-6-carboxamide 68314-31-3P, N-Allyloxy-3-(2-cyclohexylethyl)-N-Phenoxy-3H (Nees)
(HIV-integrase inhibitor; prepn. of pyrrolo[2,3-c]pyridine

(HIV-integrase inhibitor; prepn. of phydroxamates
as HIV-integrase inhibitors)
RN 688313-86-2 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide,
3-[(2,4-difluorophenyl)methyl]-Nhydroxy- (9CI) (CA INDEX NAME)

688313-90-8 CAPLUS 1H-Imidazo[4,5-c]pyridine-6-carboxamide, 4,4-difluorophenyl)methyl]-N-hydroxy- (9CI) (CA INDEX NAME)

688314-02-5 CAPLUS 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(4-fluorophenyl)methyl]-N-(phenylmethoxy)- (9CI) (CA INDEX NAME)

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Title bicyclic hydroxamate compds. I [wherein R1-R3 = independently H, CO2Rc, or (un)substituted (halo)alkyl, alkenyl, or heteroalkyl; Rc =

H, OH, alkyl, alkenyl, alkynyl, (hetero)cycloalkyl, or (un)substituted (hetero)aryl; R4 and R6 = independently H or (un)substituted (halo)alkyl, alkenyl, alkynyl, or heteroalkyl; R5 = H, (halo)alkyl, alkenyl, alkynyl, or heteroalkyl; or R4 and R6 together with the N to which R6 is attached may form a fused heterocycle; R7 = H or (un)substituted (halo)alkyl, alkenyl, heteroolkyl, or (heterolsryl; X = C or N; Y = C or N; C = C or N; Or a pharmaceutically acceptable salt, prodrug, or active metabolite thereof) were prepared as HIV-integrase inhibitors for the treatment of HIV-mediated diseases and conditions,

inhibitors for the treatment of HIV-mediated diseases and conditions, such as AIDS (no data). Examples include 31 synthetic prepns. of pyrrolo[2,3-c]pyridine hydroxamates with data, 32 addn1. prepns. of bicyclic hydroxamates without data. bicassays for HIV-integrase activity and HIV-1 cell protection without data. Por instance, Et 1H-pyrrolo[2,3-c]pyridine-5-carboxylate was coupled with 2,4-difluorobenzyl bromide using NAH in DNF to give the N-alkylated provided the acid (55%), which was treated with HONN2-HC1 in the presence of HATU and TEA to efford (2,4-difluorobenzyl)-N-hydroxy-1H-pyrrolo[2,3-c]pyridine-5-carboxamide (11) in 48% yield. (68313-66-2P, 3-(2,4-Difluorobenzyl)-N-hydroxy-1H-inidazo[4,5-c]pyridine-6-carboxamide 683313-90-8P, 1-(2,4-Difluorobenzyl)-N-hydroxy-1H-inidazo[4,5-c]pyridine-6-carboxamide 683318-07-0P, 3-(4-Pluorobenzyl)-N-menchoxy-3H-inidazo[4,5-c]pyridine-6-carboxamide 68318-07-0P, 3-(4-Pluorobenzyl)-N-menchoxy-3H-inidazo[4,5-c]pyridine-6-carboxamide 68318-09-2P, 3-(4-Pluorobenzyl)-N-phency-3H-inidazo[4,5-c]pyridine-6-carboxamide 68318-09-2P, 3-(4-Pluorobenzyl)-N-phency-3H-inidazo[4,5-c]pyridine-6-carboxamide 68318-10-5P, N-(Allyloxy)-3H-inidazo[4,5-c]pyridine-6-carboxamide 68318-10-5P, N-(Allyloxy)-3H-inidazo[4,5-c]pyridine-6-carboxamide 68318-10-5P, N-(Allyloxy)-3-(4-

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

688314-07-0 CAPLUS
3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-{(4-fluorophenyl)methyl]-N-methoxy-(9CI) (CA INDEX NAME)

688314-08-1 CAPLUS
3H-Inidazo[4,5-c]pyridine-6-carboxamide, 3-{(4-fluorophenyl)methyl]-N-phenoxy- (9C1) (CA INDEX NAME)

688314-09-2 CAPLUS
3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(4-fluorophenyl)methyl]-N[(pentafluorophenyl)methoxy]- (9CI) (CA INDEX NAME)

688314-10-5 CAPLUS
3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(4-fluorophenyl)methyl]-N-(2-propenyloxy)- (9C1) (CA INDEX NAME)

L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

H₂C= CH- CH₂-0-NH- C N N- CH₂-F

RN 688314-23-0 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide,
3-[(2,3-difluorophenyl)methyl]-Nphenoxy- (9CI) (CA INDEX NAME)

RN 688314-24-1 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide,
3-[(2,3-difluorophenyl)methyl]-Nmethoxy- (9CI) (CA INDEX NAME)

RN 688314-25-2 CAPLUS CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(2,3-difluorophenyl)methyl)-N-(2-propenyloxy)- (9CI) (CA INDEX NAME)

L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-(3-methylbutyl)-N-phenoxy(9C1) (CA INDEX NAME)

RN 688314-30-9 CAPLUS

CN 3H-Imidazo[4,5-c]pyridine-6-cerboxamide, 3-(2-cyclohexylethyl)-N-phenoxy(9C1) (CA INDEX NAME)

RN 688314-31-0 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-{2-cyclohexylethyl}-N-methoxy(9CI) (CA INDEX NAME)

RN 688314-32-1 CAPLUS CN 3H-Imidsac(4,5-c|pyridine-6-carboxamide, 3-(2-cyclohexylethyl)-N-(2-propenyloxy)- (9CI) (CA INDEX NAME)

L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 688314-26-3 CAPLUS
CN 1H-Imidazo[4,5-c]pyridine-6-carboxamide, 1-[(4-fluorophenyl)methyl]-N-phenoxy- (9CI) (CA INDEX NAME)

RN 688314-27-4 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide,
3-[(2,3-difluorophenyl)methyl]-N[1,1-dimethylethoxyl- (9CI) (CA INDEX NAME)

RN 688314-28-5 CAPLUS
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, N-methoxy-3-(3-methylbutyl)(9CI) (CA INDEX NAME)

RN 688314-29-6 CAPLUS

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N
O

112
13
14
0
15

chain nodes :

12 13 14 15 18 20 21 24

ring nodes :

1 2 3 4 5 6 7 8 9 10 22 23

chain bonds :

2-18 9-20 10-21 12-13 13-14 13-15 22-24

ring bonds :

1-2 1-5 2-3 3-4 4-6 4-5 5-9 6-7 6-23 7-8 7-10 8-9 10-22 22-23

exact/norm bonds :

1-2 1-5 2-3 2-18 3-4 4-6 4-5 5-9 6-7 6-23 7-8 7-10 8-9 9-20 10-21

10-22 13-14 13-15 22-23 22-24

exact bonds :

12-13

isolated ring systems :

containing 1 :

G1:H,[*1]

G2:H,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

12:CLASS 13:CLASS 14:CLASS 15:CLASS 18:CLASS 20:CLASS 21:CLASS 22:Atom

23:Atom 24:CLASS

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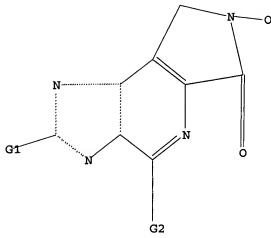
STR

=> d

L4 HAS NO ANSWERS

L4

Page 13



0

G1 H, [@1]

G2 H, Ak

Structure attributes must be viewed using STN Express query preparation.

=> s 14 ful

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 06:13:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 35 TO ITERATE

100.0% PROCESSED

35 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L5

0 SEA SSS FUL L4

L6

0 L5

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chain nodes : 11 14 15 16 17 18 21 23 ring nodes : 1 2 3 4 5 6 7 8 9 ring/chain nodes : 10 12 chain bonds : 2-21 7-10 9-23 10-11 10-12 12-14 15-16 16-17 16-18 ring bonds : 1-2 1-5 2-3 3-4 4-6 4-5 5-9 6-7 7-8 8-9 exact/norm bonds : 1-2 1-5 2-3 2-21 3-4 4-6 4-5 5-9 6-7 7-8 8-9 9-23 10-11 10-12 12-14 16-17 16-18 exact bonds : 7-10 15-16 isolated ring systems : containing 1 :

G1:H,[*1]

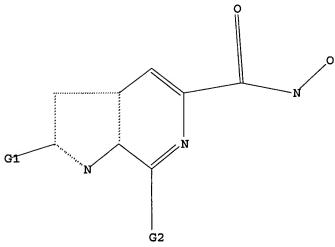
G2:H,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 21:CLASS 23:CLASS

L7 STRUCTURE UPLOADED

=> d L7 HAS NO ANSWERS L7 STR



0

G1 H, [@1] G2 H, Ak

Structure attributes must be viewed using STN Express query preparation.

=> s 17 ful

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 06:15:25 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1216 TO ITERATE

100.0% PROCESSED 1216 ITERATIONS

202 ANSWERS

SEARCH TIME: 00.00.02

202 SEA SSS FUL L7

L9 4 L8

=> d fbib abs

L8

L9

ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
yield. The invented compde. are useful for the treatment of diseases
mediated by HIV, such as AIDS and AIDS related complex.
CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT.

```
L9 ANSMER 1 OP 4 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2006:237568 CAPLUS
DN 144:312070
TI Preparation of N-hydroxy pyrrolopyridinecarboxamides as inhibitors of HIV integrate.
IN Dress, Klaus; Kuehler, Jon Edward; Plewe, Michael Bruno; Yang, Anle; Zhang, Junhu
PA Pfizer Inc., USA
PCODEN: PIXXD2
TP Attent
LA English
PAN.CNT 1
PATENT NO. KIND DATE APPLICATION NO. DATE

PI WO 2005027694 A1 20060316 WO 2005-182967 20050826
M: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BM, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HB, HU, ID, LI, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LE, LT, LU, LV, MA, MD, MG, MK, MN, MM, MK, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SI, SM, ST, JJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZM
RM: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CP, CG, CI, CM, AG, AG, NG, GG, MM, MR, KE, SN, TD, TO, BM, GH, GM, KE, LS, MM, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZM, AM, AZ, BY, KG, KI
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AB Title compds. I (wherein R1, R6 = H, (substituted) alkyl, alkenyl, etc.; R2, R5 = H; R3 = pyrrolidinylmethyl, piperidinylmethyl, etc.; R4 = H, halo, alkyl, etc.; R7 = H, heteroslkyl, aryl, etc.] and pharmaceutically acceptable salts and solvates thereof were prepared as inhibitors of HIV integrase. For instance, condensation of Me Seter II (R = OME) with hydroxylamine at ambient temperature gave hydroxyamide II (R = NHOH) in

Page 16

```
ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
2005:1171056 CAPLUS
143:440391
Preparation of N-hydroxy pyrrolopyrimidinecarboxamides as inhibitors of
HIV integrase.
Dress, Klaus Ruprecht; Hu, Qiyue; Johnson, Ted William; Plewe, Michael
Bruno; Tanis, Steven Paul; Wang, Hai; Yang, Anle; Yin, Chunfeng; Zhang,
Junhu
Pfizer Inc., USA
PCT Int. Appl., 177 pp.
CODEN: PIXD2
Patent
English
.CNT 1
PATENT NO. KIND DATE APPLICATION NO. DATE
IN
                           PATENT NO. KIND DATE APPLICATION NO. DATE

WO 20051031031 A2 20051103

WI: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BM, BY, BZ, CA, CH, CM, CC, CC, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GB, GH, UM, HR, HU, LD, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MM, MM, KM, MX, MX, MX, NN, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TM, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZM

RWI: BM, GH, GM, KE, LS, MM, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZM, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, CB, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BP, BJ, CP, CG, CI, CM, GA, GM, GQ, GW, ML, MR, NR, NE, SN, TD, TG

WS 2004-56570SP P 20040426
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US 2005-660502P
US 2005-115003
US 2004-565705P
US 2005-660502P
                                                                                                                                                                                                                                                                                                                                                                                                                   P 20040426
P 20050309
20050425
P 20040426
P 20050309
                               US 2005277662
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                              MARPAT 143:440391
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Title compds. [I; R1 = H, (substituted) alkyl, alkenyl, heteroalkyl; R2, R5 = H; R3 = (CRBR9):NRIORN1, (substituted) heteroalkyl; R4 = H, halo, alkyl, heteroalkyl, (substituted) alkenyl, alkynyl, OR12a, NR12aR12b; R6

H, alkyl, heteroalkyl, (substituted) alkenyl; R8, R9 = H, alkyl; R10R11N

ANSMER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) (substituted) cycloheteroalkyl; R12a, R12b, R12c = H, alkyl; t = 1-3], were prepd. Thus, 1-(2,4-diffluorobenzyl)-1H-pyrrolo[2,3-c)pyridine-5-carboxylic acid (prepn. given) was stirred with -azabenzotrizacol-1-yl)1,1,3,3-tetramethyluronium hexafluorophosphate, Et3N, and NH2OH.HCl in

for 16 h to give 48% N-hydroxy-1-(2,4-difluorobenzyl)-1H-pyrrolo(2,3-c)pyridine-5-carboxamide. The latter showed an EC50 = 0.00795 μM in an HIV-1 cell protection assay.

R3 Z-N 0

AB Title compds. [1; R1 = H, (substituted) alkyl, alkenyl, heteroalkyl; R2 = H, alkyl; R3 = H, alkyl, (substituted) heteroalkyl, aminoalkyl, aminoarbonyl, etc.; Z = (C(R4)21n, CR4:CR4, etc.; R4 = H, halo,

L9 ANSMER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
heteroalkyl, (substituted) alkyl, cycloslkyl, sryl, heteroalkyl,
cycloheteroalkyl; R5 = H, heteroalky, aryl, alkenyl, (substituted) alkyl;
R6 = H; n = 1-4), were prepd. Thus, 3-(4-fluorobenzyl)-7-hydroxy-3,7dihydro-6H-pyrrolo[2,3-c]-1,7-naphthyridin-6-one (multistep prepn. given)
showed ECSO = 0.4 mM in an HIV-1 cell protection assay.

RE.CNT 6 THER ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB Title bicyclic hydroxamate compds. I [wherein R1-R3 = independently H, COURC, or (un)eubstituted (halo)alkyl, alkenyl, or heteroalkyl; Rc = halo,
H, OH, alkyl, alkenyl, alkynyl, (hetero)cycloalkyl, or (un)substituted (heterolaryl; RA and R6 = independently H or (un)eubstituted (halo)alkyl, alkenyl, alkynyl, or heteroalkyl; RC = halo,
alkenyl, alkynyl, or heteroalkyl; RS = H, (halo)alkyl, alkenyl, alkynyl, or R4 and R6 together with the N to which R6 is attached may form a fused heterocycle; R7 = H or (un)substituted (halo)alkyl, alkenyl, alkynyl, heteroalkyl; cor N; Y = C or N; Y = C or N; Or a pharmaceutically acceptable salt, prodrug, or active metabolite thereof) were prepared as HIV-integrase einhibitors for the treatment of HIV-mediated diseases and conditions, such as AIDS (no data). Examples include 31 synthetic prepns. of pyrrolo(2,3-clpyridine-5-carboxylate was coupled with 2,4-difluorobenzyl bromide using NaH in DMP to give the N-alkylated pyrrolopyridinecarboxylate (481). Saponification with NaOH in MeOM provided the acid (558), which was treated with HONH2=HCl in the presence of HATU and TEA to afford

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chain nodes :

11 14 15 16 17 18 21 23

ring nodes :

1 2 3 4 5 6 7 8 9

ring/chain nodes :

10 12

chain bonds :

2-21 7-10 9-23 10-11 10-12 12-14 15-16 16-17 16-18

ring bonds :

1-2 1-5 2-3 3-4 4-6 4-5 5-9 6-7 7-8 8-9

exact/norm bonds :

1-2 2-3 2-21 3-4 4-6 4-5 5-9 6-7 7-8 8-9 9-23 10-11 10-12 12-14 16-17

16-18

exact bonds :

1-5 7-10 15-16

isolated ring systems :

containing 1:

G1:H,[*1]

G2:H,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 21:CLASS

23:CLASS

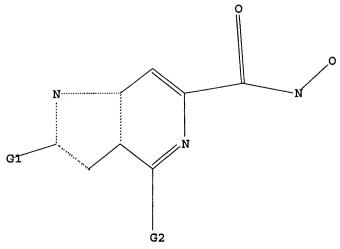
L10 STRUCTURE UPLOADED

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L10 HAS NO ANSWERS

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G1 H, [@1] G2 H, Ak

Structure attributes must be viewed using STN Express query preparation.

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Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

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SCREENING

FULL SCREEN SEARCH COMPLETED -

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12 ANSWERS

100.0% PROCESSED 1028 ITERATIONS

SEARCH TIME: 00.00.31

L11 12 SEA SSS FUL L10

L12 2 L11

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L12 ANSMER 1 OP 2 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:1171056 CAPLUS
DN 143:440391
TI Preparation of N-hydroxy pytrolopyrimidinecerboxamides as inhibitors of
HIV integrase.
IN Dress, Klaus Ruprecht; Hu, Qiyue; Johnson, Ted Milliam; Plewe, Michael
Bruno; Tanis, Steven Paul; Mang, Hai; Yang, Anle; Yin, Chunfeng; Zhang,
Junhu
PA Pfizer Inc., USA
SO PCT Int. Appl., 177 pp.
COOEN: PIXXD2
DT Patent
LA English
PAN.CNT 1
PATENT NO. KIND DATE APPLICATION NO. DATE
                               CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

MO 2005103003 A3 20051103 MO 2005-1B1029 20050414

MO 2005103003 A3 20060316

M1 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BM, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GB, GH, GM, HR, HU, ID, IL, IN, IS, JP, KB, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MN, MX, MZ, NA, N1, NO, NZ, GM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, ZM, TM, TM, TM, TM, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZM, ZM, GM, GM, GM, KE, LS, MM, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZM, AM, AZ, BY, NG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BP, BJ, CF, CG, CI, CM, GA, GN, GG, GM, ML, MR, NE, SN, TD, TG

US 2004-565705P P 20040414
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US 2005-660502P
US 2005-115003
US 2004-565705P
US 2005-660502P
                                    US 2005277662
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                                    MARPAT 143:440391
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Title compds. [I; Rl = H, (substituted) alkyl, alkenyl, heteroalkyl; R2, R5 = H; R3 = (CR8R9)tNR10R11, (substituted) heteroalkyl; R4 = H, halo, alkyl, heteroalkyl, (substituted) alkenyl, alkynyl, OR12a, NR12aR12b; R6 AB

H, alkyl, heteroalkyl, (substituted) alkenyl; R8, R9 = H, alkyl; R10R11N

- L12 ANSMER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) (substituted) cycloheteroelkyl; R12a, R12b, R12c = H, alkyl; t = 1-3], were prepd. Thus, 1-(2,4-difluorobenzyl)-1H-pyrrolo[2,3-c]pyridine-5-carboxylic acid (prepn. given) was stirred with (-(7-axabenzotrizol-1-yl)- [1,1,3,3-tetramethyluronium hexafluorophosphate, Et3N, and NH2OH.HCl in
- - for 16 h to give 48% N-hydroxy-1-(2,4-difluorobenzyl)-1H-pyrrolo[2,3-c]pyridine-5-carboxamide. The latter showed an EC50 = 0.00795 µM in an HIV-1 cell protection assay.

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ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
2004:390246 CAPLUS
140:406796
Preparation of pyrrolo[2,3-c]pyridine hydroxamates as HIV-integrase inhibitors
HU, Qiyue; Kuki, Atsuo; Nowlin, Dawn Marie; Plewe, Michael Bruno; Wang, Hai; Zhang, Junhu
Pfizer Inc. USA
PCT Inc. Appl., 108 pp.
CODEN: PIXXD2
Patent
English
CNT 1
PATENT NO. KIND DATE APPLICATION NO. DATE
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SO
                                                        MO 2004039803

NO 2004039803

NO 2004039803

NO AE, AG, AL,
CO, CR, CU,
GM, HR, HU,
LS, LT, LU,
PH, PL, PT,
TZ, LA, UG,
RW: GH, GM, KE,
KG, KZ, MD,
FI, FR, GB,
BP, BJ, CP,
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            AU 2003269421
                             AT, BE, CH, DE, DK, ES, FR, GB,
IE, SI, LT, LV, FI, RO, MK, CY,
            BR 2003015820
            JP 2006506398
            US 2004147547
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20051214
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                                                                                                                                                           P 20021031
           MARPAT 140:406796
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L12 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) 11

Title bicyclic hydroxamate compds. I [wherein R1-R3 = independently H, CO2Rc, or (un)substituted (halo)alkyl, alkenyl, or heteroalkyl; Rc =

H, OH, alkyl, alkenyl, alkynyl, (hetero)cycloalkyl, or (un)substituted (hetero)aryl; R4 and R6 = independently H or (un)substituted (halo)alkyl, alkenyl, alkynyl, or heteroalkyl; R5 = H, (halo)alkyl, alkenyl, alkynyl, or heteroalkyl; cr R4 and R6 together with the N to which R6 is attached may form a fused heterocycle; R7 = H or (un)substituted (halo)alkyl, alkenyl, heteroalkyl, or (heterolaryl; X = C or N; Y = C or N; C = C or N; Or a pharmaceutically acceptable salt, prodrug, or active metabolite thereof) were prepared as HIV-integrase inhibitors for the treatment of HIV-mediated diseases and conditions,

as AIDS (no data). Examples include 31 synthetic prepns. of pyrrolo[2,3-c]pyridine hydroxamates with data, 32 addnl. prepns. of bicyclic hydroxamates without data, bicassays for HIV-integrase activity and HIV-1 cell protection without data. For instance, Et IH-pyrrolo[2,3-c]pyridine-5-carboxylate was coupled with 2,4-difluorobensyl bromide using NaH in DMF to give the N-alkylated pyrrolopyridinecarboxylate (48%). Saponification with NaOH in MeOH provided the acid (55%), which was treated with HONN2-HCl in the presence of HATU and TEA to afford (2,4-difluorobensyl)-N-hydroxy-IH-pyrrolo[2,3-c]pyridine-5-carboxamide (II) in 48% yield.